1(3H)-Isobenzofuranone, 3,3-dimethyl-

Other names:	1,3-2H-Isobenzofuranone, 3,3-dimethyl- 3,3-dimethylphthalide
Inchi:	InChI=1S/C10H10O2/c1-10(2)8-6-4-3-5-7(8)9(11)12-10/h3-6H,1-2H3
InchiKey:	YFBZUWUJSCLVST-UHFFFAOYSA-N
Formula:	C10H10O2
SMILES:	CC1(C)OC(=O)c2ccccc21
Mol. weight [g/mol]:	162.19
CAS:	1689-09-4

Physical Properties

Property code	Value	Unit	Source
gf	-17.35	kJ/mol	Joback Method
hf	-206.33	kJ/mol	Joback Method
hfus	14.63	kJ/mol	Joback Method
hvap	48.31	kJ/mol	Joback Method
log10ws	-2.58		Crippen Method
logp	2.092		Crippen Method
mcvol	124.580	ml/mol	McGowan Method
pc	3624.61	kPa	Joback Method
tb	561.61	K	Joback Method
tc	809.29	K	Joback Method
tf	378.03	K	Joback Method
vc	0.470	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	297.30	J/mol×K	561.61	Joback Method
cpg	311.23	J/mol×K	602.89	Joback Method
cpg	324.18	J/mol×K	644.17	Joback Method
cpg	336.32	J/mol×K	685.45	Joback Method
cpg	347.82	J/mol×K	726.73	Joback Method
cpg	358.84	J/mol×K	768.01	Joback Method
cpg	369.53	J/mol×K	809.29	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1689094&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume